

**Supplemental material for:**

**Metabolic modelling reveals broad changes in gut microbial metabolism in inflammatory bowel disease patients with dysbiosis**

Almut Heinken<sup>1,2</sup>, Johannes Hertel<sup>1,2,3</sup>, and Ines Thiele<sup>1,2,4,5\*</sup>

<sup>1</sup> School of Medicine, National University of Ireland, Galway, University Road, Galway, Ireland

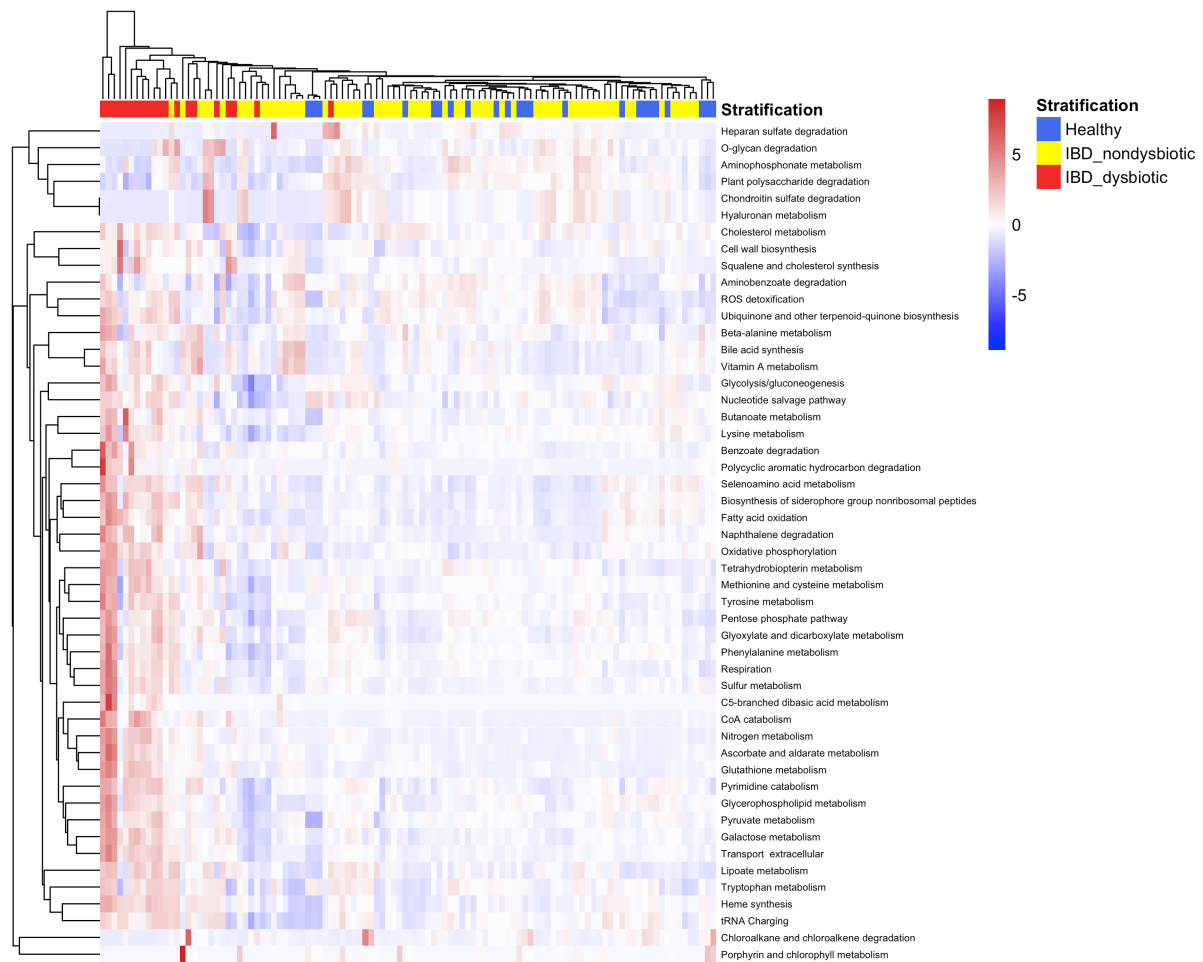
<sup>2</sup> Ryan Institute, National University of Ireland, Galway, Galway, Ireland

<sup>3</sup> Department of Psychiatry and Psychotherapy, University Medicine Greifswald, Greifswald, Germany

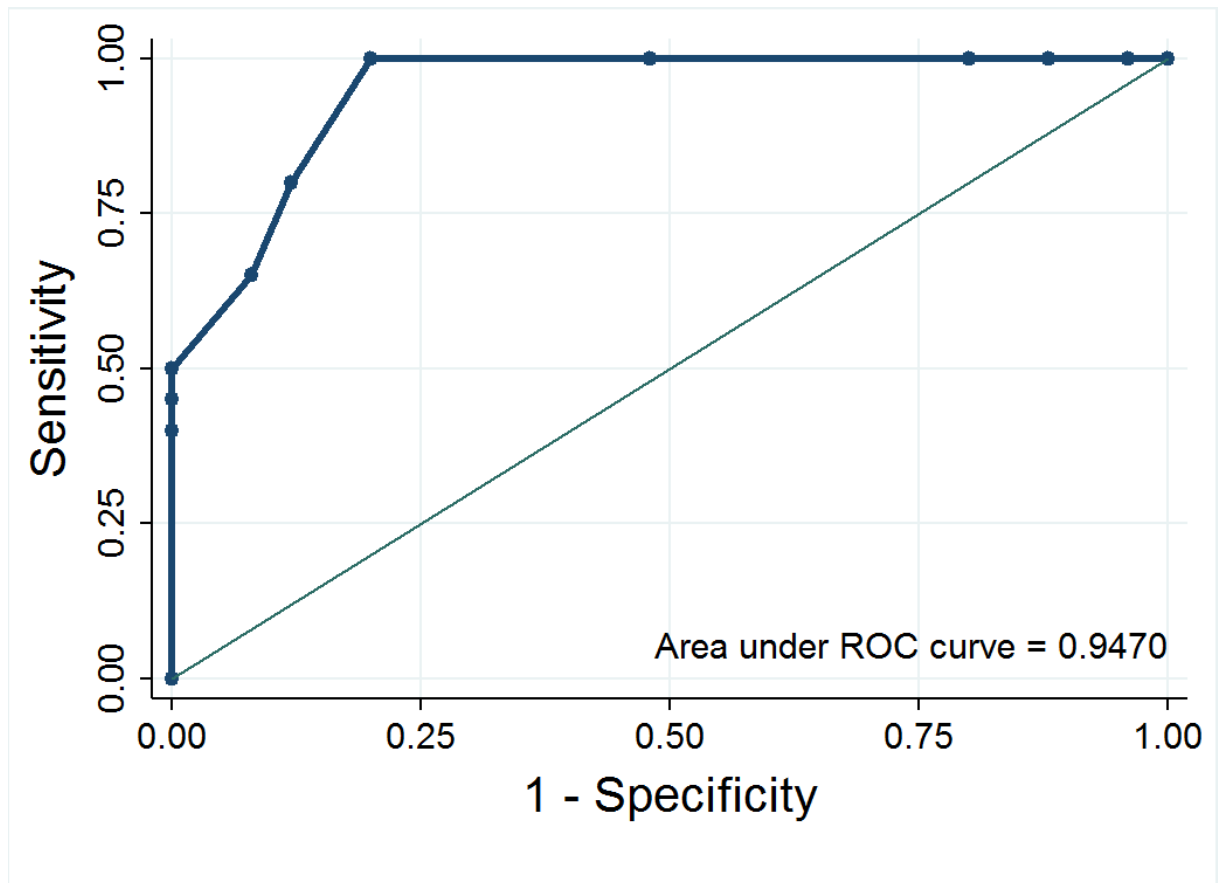
<sup>4</sup> Division of Microbiology, National University of Galway, Galway, Ireland

<sup>5</sup> APC Microbiome Ireland, Cork, Ireland

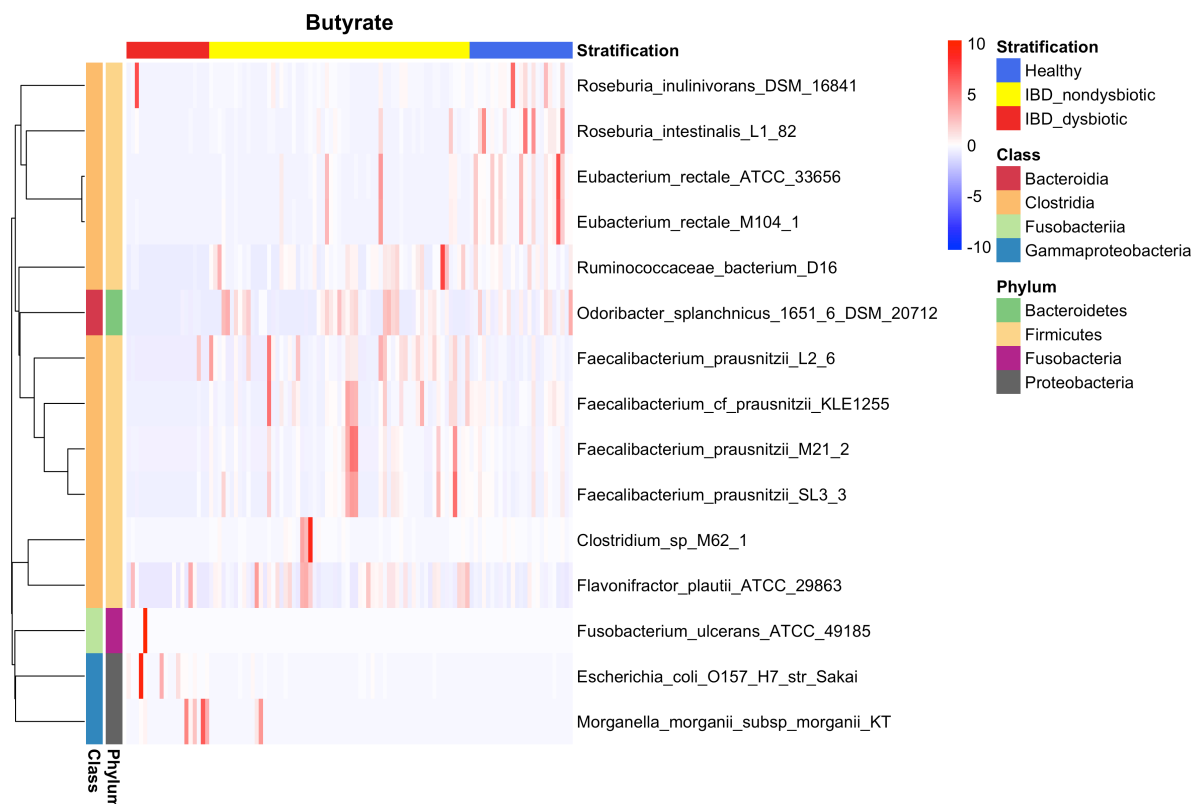
\*Corresponding author: Ines Thiele, School of Medicine, National University of Ireland, Galway, University Road, Galway, Ireland. Email: [ines.thiele@nuigalway.ie](mailto:ines.thiele@nuigalway.ie)



**Supplementary Figure 1:** Quantitative abundances of pathways in the 108 microbiomes. Shown are all subsystems that, after summarizing abundances for the corresponding reactions, were significantly different between healthy and IBD and/or between the dysbiotic and non-dysbiotic IBD cluster after correcting for false discovery rate.

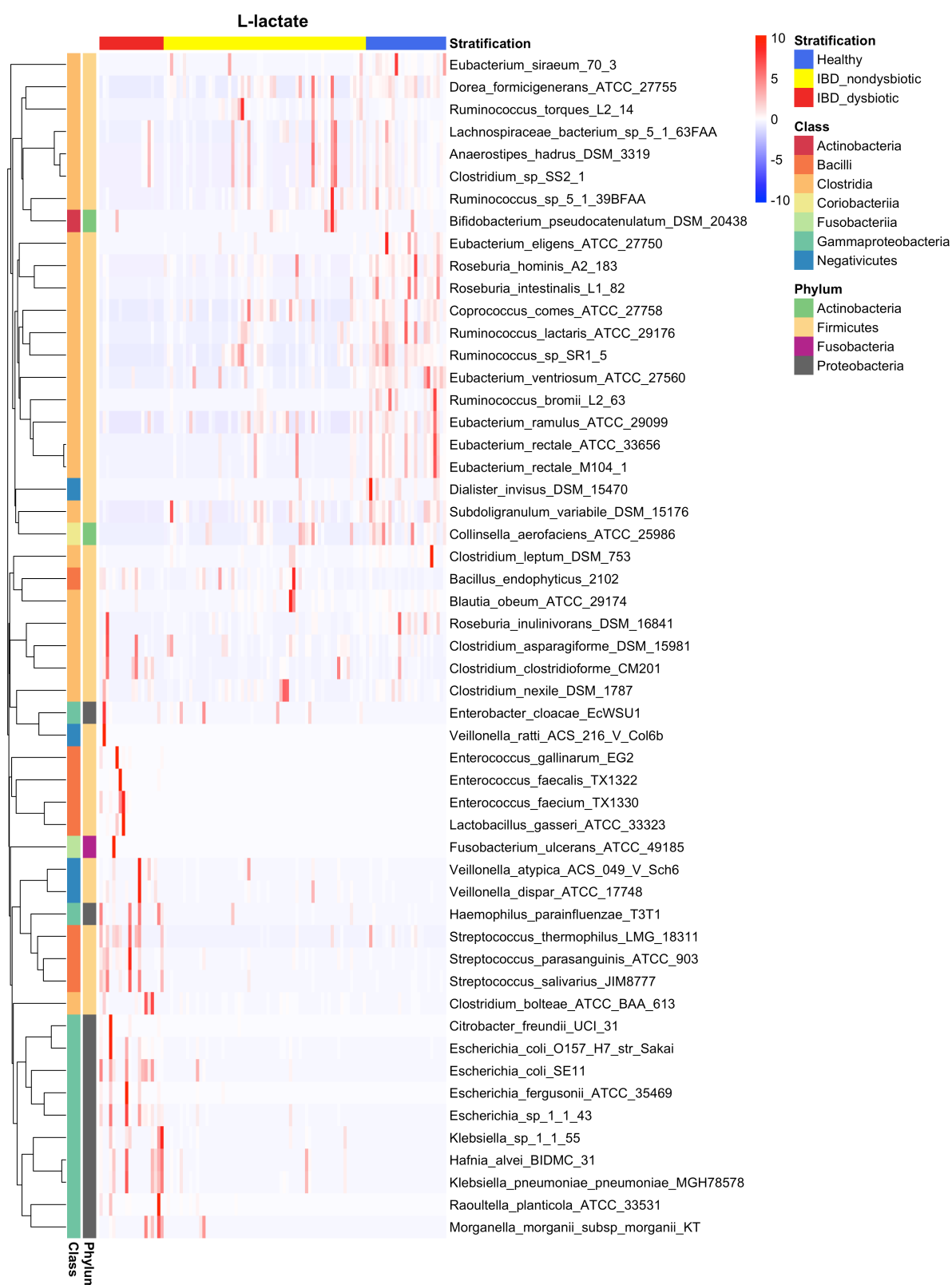


**Supplementary Figure 2:** AUC from logistic regression, classifying healthy individuals using the number of independently secreted sulphur metabolites as only predictor. AUC is significantly bigger than 0.5,  $p=0.003$ .



**Supplementary Figure 3:** Strain-level contributions to total butyrate production (mmol/person/day) in all 108 personalised microbiome models.

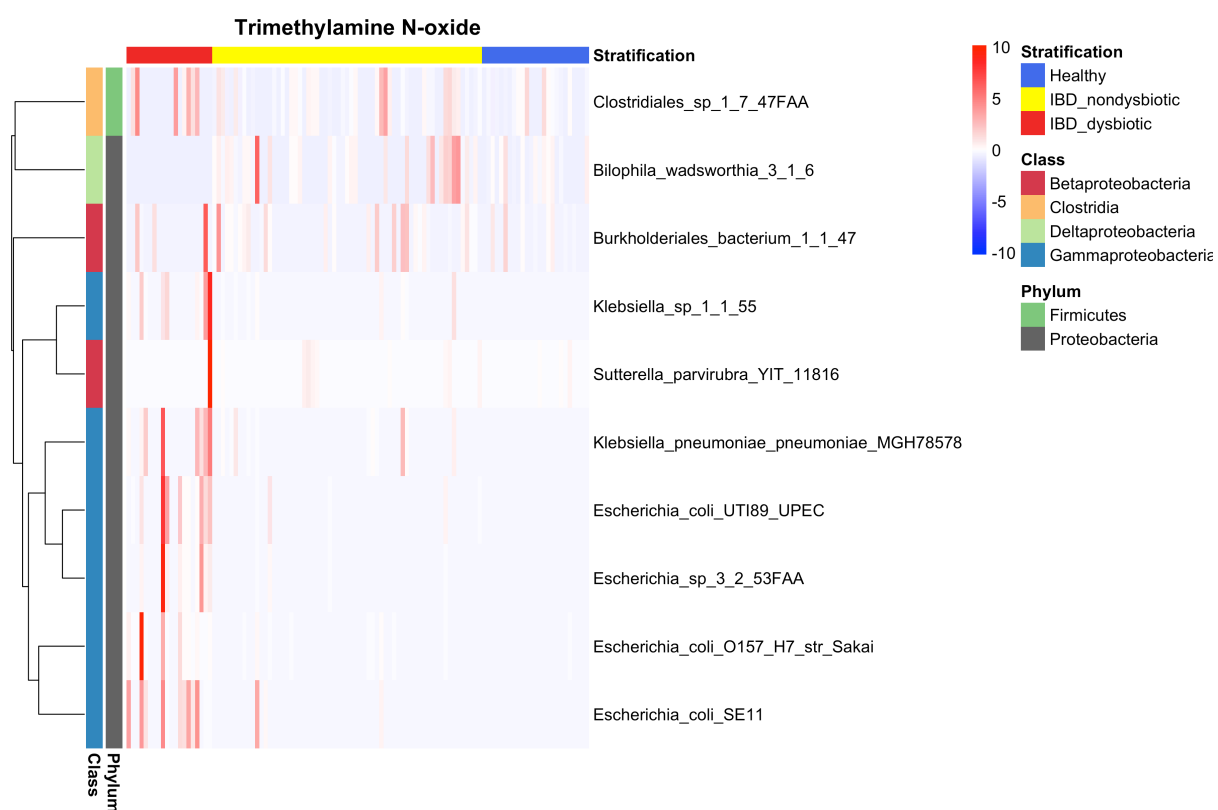




**Supplementary Figure 4:** Strain-level contributions to total L-lactate production (mmol/person/day) in all 108 personalised microbiome models.



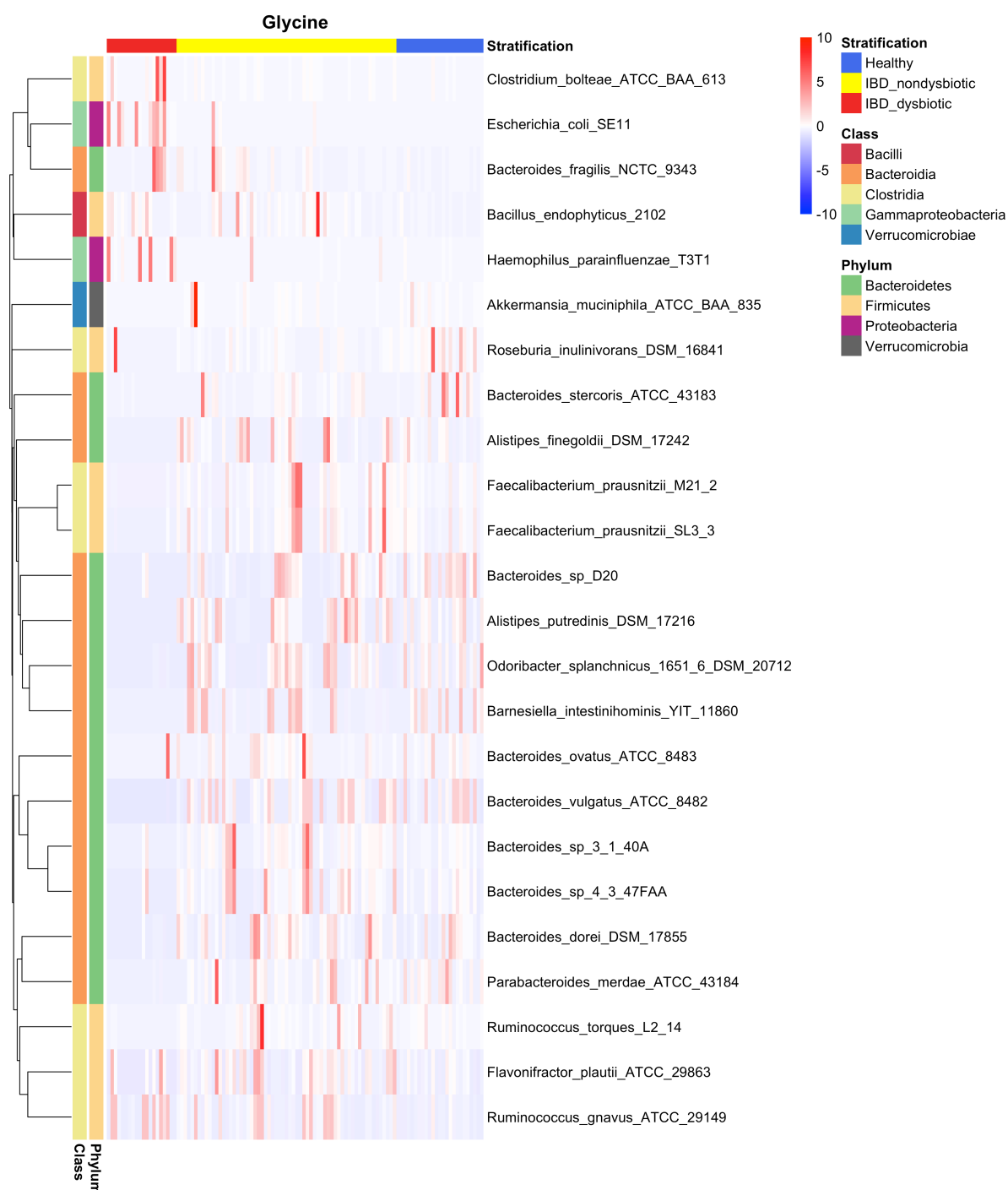
**Supplementary Figure 5:** Strain-level contributions to total hydrogen sulphide production (mmol/person/day) in all 108 personalised microbiome models.



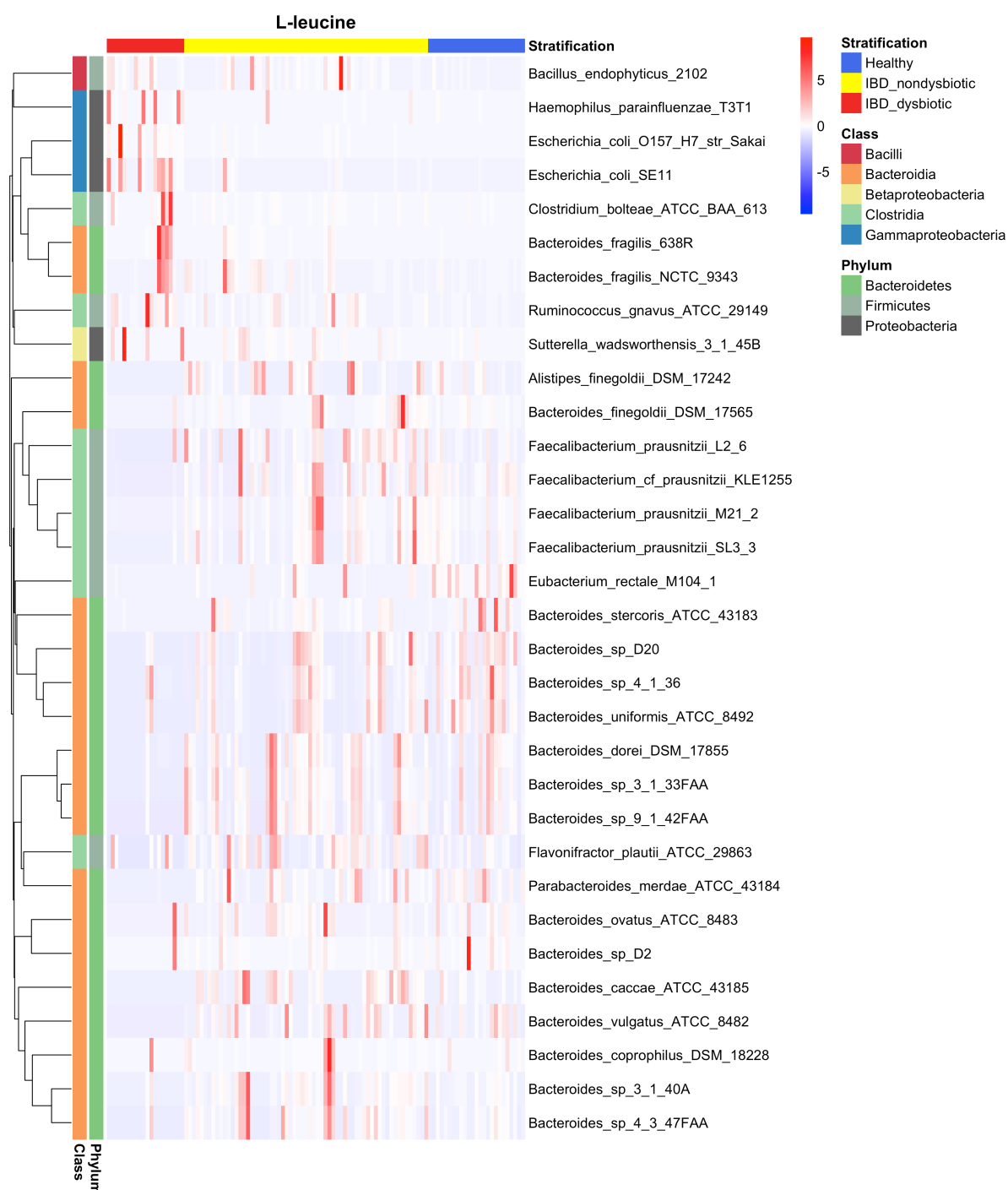
**Supplementary Figure 6:** Strain-level contributions to total trimethylamine-N-oxide production (mmol/person/day) in all 108 personalised microbiome models.



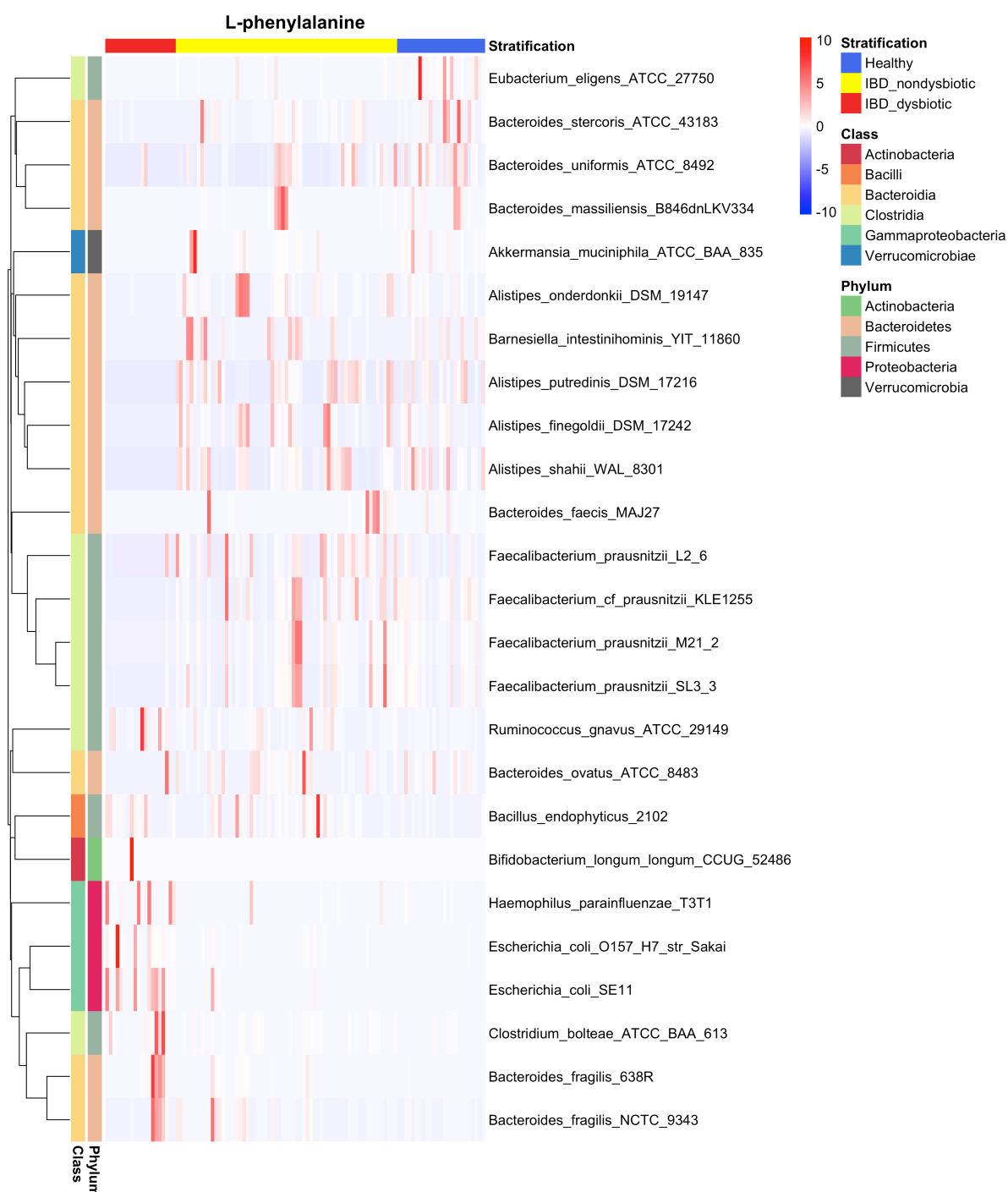
**Supplementary Figure 7:** Strain-level contributions to total nicotinamide production (mmol/person/day) in all 108 personalised microbiome models.



**Supplementary Figure 8:** Strain-level contributions to total glycine production (mmol/person/day) in all 108 personalised microbiome models.



**Supplementary Figure 9:** Strain-level contributions to total L-leucine production (mmol/person/day) in all 108 personalised microbiome models.

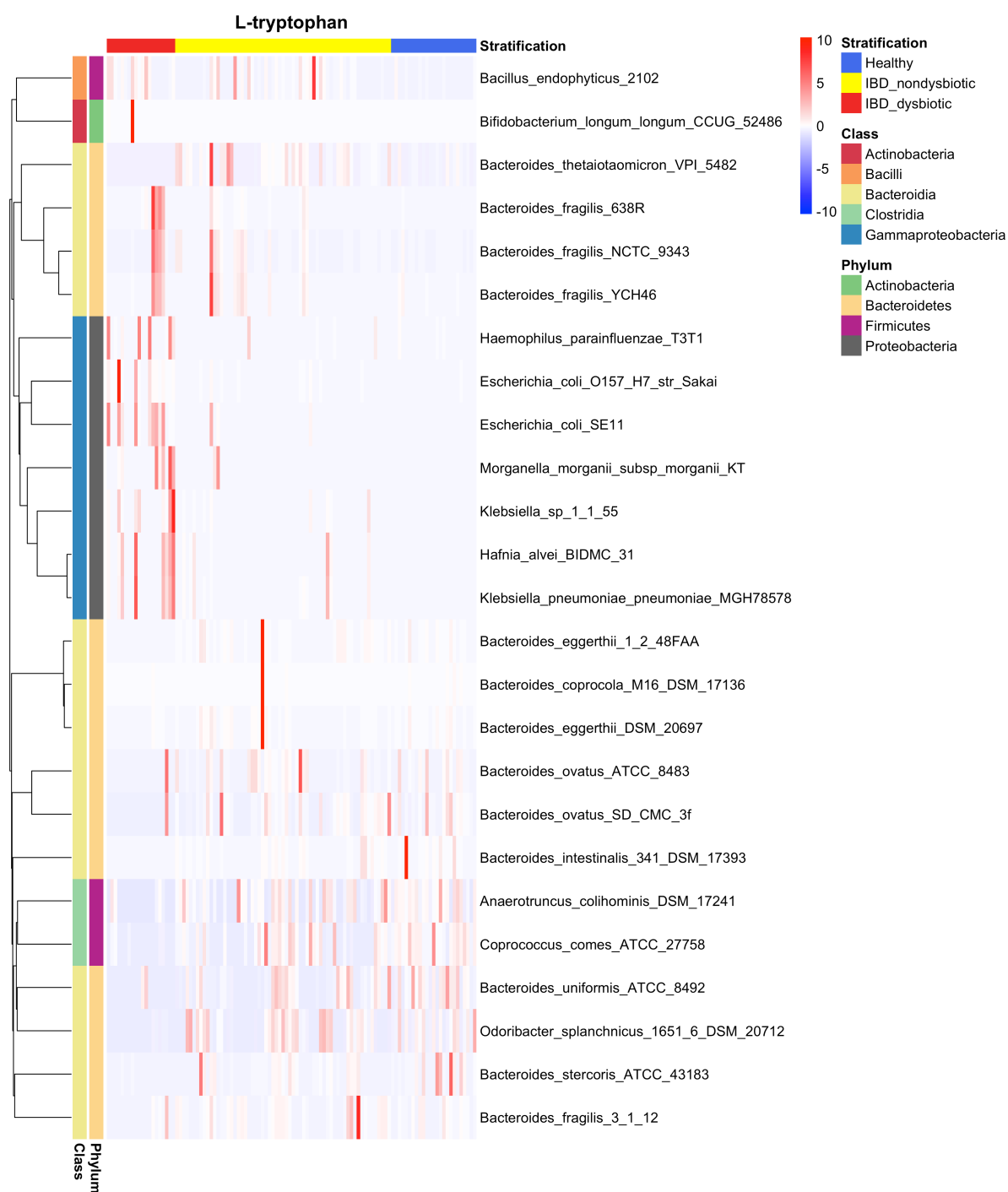


**Supplementary Figure 10:** Strain-level contributions to total L-phenylalanine production (mmol/person/day) in all 108 personalised microbiome models.



**Supplementary Figure 11:** Strain-level contributions to total L-tyrosine production (mmol/person/day) in all 108 personalised microbiome models.





**Supplementary Figure 12:** Strain-level contributions to total L-tryptophan production (mmol/person/day) in all 108 personalised microbiome models.